INFRARED SPECTROSCOPY OF TITANIUM CATION ACETYLENE COMPLEXES: CATION-π COMPLEXES VS REACTED STRUCTURES

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Titanium cation-acetylene complexes are investigated with infrared photodissociation spectroscopy to study latent reactivity. $Ti^+(C_2H_2)_n$ complexes are produced via laser vaporization of a titanium rod in a supersonic expansion of argon containing acetylene. Argon-tagged complexes are mass selected in a time-of-flight mass spectrometer and their spectra are measured in the C-H stretching region with infrared laser photodissociation. These spectra are assigned with the aid of B3LYP/Def2TZVP computations. The presence of reacted structures and cation-π structures is investigated by comparing experiment to theory.